Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2-Chlorothiazol-5-yl)methyl 4-nitrophenyl carbonate

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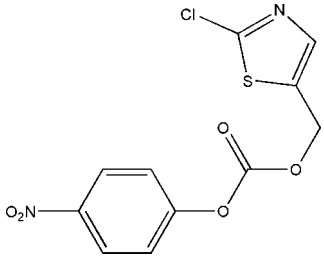
Received 30 October 2007; accepted 2 November 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.052; wR factor = 0.159; data-to-parameter ratio = 14.0.

In the molecule of the title compound, $C_{11}H_7ClN_2O_5S$, the benzene and thiazole rings are oriented at a dihedral angle of 56.52 (3)°. In the crystal structure, intermolecular C—H···O and C—H···N hydrogen bonds link the molecules.

Related literature

For related literature, see: Kempf *et al.* (1998); Sicker (1989). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_7ClN_2O_5S$
M_r = 314.70
Monoclinic, $P2_1/c$
a = 9.7380 (19) Å
b = 10.717 (2) Å
c = 13.197 (3) Å
β = 109.17 (3)°
V = 1300.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 294 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–onius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.871, T_{max} = 0.954
2692 measured reflections
2539 independent reflections
1581 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.159
S = 1.02
2539 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O4^{i}	0.97	2.44	3.392 (4)	166
C8—H8B···N2^{ii}	0.97	2.54	3.325 (5)	138

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2361).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Kempf, D. J., Sham, H. L., Marsh, K. C., Flentge, C. A., Betebenner, D., Green, B. E., McDonald, E., Vasavanonda, S., Saldivar, A., Wideburg, N. E., Kati, W. M., Ruiz, L., Zhao, C., Fino, L. M., Patterson, J., Molla, A., Plattner, J. J. & Norbeck, D. W. (1998). *J. Med. Chem.* **41**, 602–617.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sicker, D. A. (1989). *Synthesis*, **11**, 875–876.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

  doi:10.1107/S1600536807055420

supplementary materials

Acta Cryst. (2007). E**63**, o4624 [**doi:10.1107/S1600536807055420**]

(2-Chlorothiazol-5-yl)methyl 4-nitrophenyl carbonate

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Comment

The title compound, (I), is one of the aromatic carbonates, which are an important class of esters compounds and have widespread applications from pharmaceuticals (Kempf *et al.*, 1998) to agronomy (Sicker, 1989). As part of our studies in this area, we report herein the synthesis and crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6) and B (C9/C10/N2/C11/S) are, of course, planar and they are oriented at a dihedral angle of 56.52 (3)°.

In the crystal structure, intermolecular C—H···O and C—H···N hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, (I), a solution of 2-chloro-5 -(hydroxymethyl)thiazole (1.5 g, 10 mmol) and excess *N*-methyl morpholine in methylene chloride (50 ml) was cooled to 273 K, and treated with 4-nitophenyl chloroformate (3.0 g, 15 mmol). After being stirred for 6 h, the reaction mixture was diluted with $CHCl_3$, washed successively with 1 N HCl, saturated aqueous $NaHCO_3$, and saturated bine, dried over $NaSO_4$, and concentrated *in vacuo*. The residue was recrystallized by methylene chloride to give the title compound, (I) (yield; 2.6 g, 82%). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methyl H, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

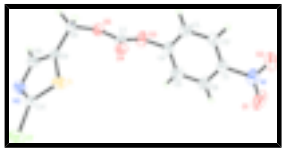

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

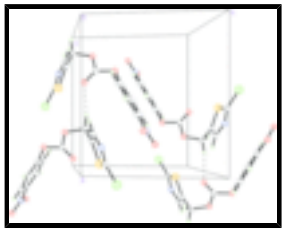

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

(2-Chlorothiazol-5-yl)methyl 4-nitrophenyl carbonate

Crystal data

$C_{11}H_7ClN_2O_5S$	$F_{000} = 640$
$M_r = 314.70$	$D_x = 1.607$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 375(2) K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.7380$ (19) Å	Cell parameters from 25 reflections
$b = 10.717$ (2) Å	$\theta = 9$–14º
$c = 13.197$ (3) Å	$\mu = 0.47$ mm^{-1}
$\beta = 109.17$ (3)º	$T = 294$ (2) K
$V = 1300.9$ (5) Å^3	Block, colorless
$Z = 4$	0.30 × 0.10 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer	$R_{int} = 0.032$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0$º
Monochromator: graphite	$\theta_{min} = 2.2$º
$T = 294(2)$ K	$h = -11 \rightarrow 11$
$\omega/2\theta$ scans	$k = 0 \rightarrow 13$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 16$
$T_{min} = 0.871$, $T_{max} = 0.954$	3 standard reflections
2692 measured reflections	every 120 min
2539 independent reflections	intensity decay: none
1581 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.159$	$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 0.3P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
2539 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
181 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl	0.24960 (15)	1.05190 (11)	0.01610 (10)	0.0831 (4)
S	0.15104 (13)	0.93594 (9)	0.18446 (8)	0.0600 (3)
O1	−0.5209 (5)	1.3043 (4)	0.4410 (3)	0.1144 (14)
O2	−0.4109 (4)	1.2199 (3)	0.5931 (3)	0.0860 (10)
O3	−0.2637 (3)	0.8347 (2)	0.2886 (2)	0.0632 (7)
O4	−0.0348 (3)	0.9101 (2)	0.33757 (19)	0.0497 (6)
O5	−0.1038 (3)	0.7334 (2)	0.2417 (2)	0.0549 (7)
N1	−0.4482 (4)	1.2216 (4)	0.4954 (3)	0.0667 (10)
N2	0.1425 (4)	0.8250 (3)	0.0107 (2)	0.0581 (8)
C1	−0.4004 (4)	1.1203 (4)	0.4410 (3)	0.0529 (9)
C2	−0.3176 (4)	1.0258 (4)	0.5019 (3)	0.0548 (9)
H2B	−0.2938	1.0261	0.5761	0.066*
C3	−0.2704 (4)	0.9307 (4)	0.4510 (3)	0.0552 (9)
H3A	−0.2147	0.8656	0.4904	0.066*
C4	−0.3069 (4)	0.9335 (3)	0.3415 (3)	0.0514 (9)
C5	−0.3905 (4)	1.0269 (4)	0.2806 (3)	0.0626 (11)
H5A	−0.4142	1.0262	0.2063	0.075*
C6	−0.4390 (4)	1.1221 (4)	0.3310 (3)	0.0622 (11)
H6A	−0.4967	1.1860	0.2914	0.075*
C7	−0.1240 (4)	0.8346 (3)	0.2937 (3)	0.0470 (8)
C8	0.0458 (4)	0.7103 (3)	0.2462 (3)	0.0544 (10)
H8A	0.0572	0.6223	0.2337	0.065*
H8B	0.1109	0.7304	0.3175	0.065*
C9	0.0881 (4)	0.7848 (3)	0.1659 (3)	0.0439 (8)
C10	0.0921 (4)	0.7439 (3)	0.0710 (3)	0.0505 (9)
H10A	0.0619	0.6637	0.0468	0.061*
C11	0.1761 (4)	0.9284 (3)	0.0624 (3)	0.0510 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0979 (9)	0.0693 (7)	0.0924 (9)	−0.0089 (6)	0.0452 (7)	0.0247 (6)

S	0.0931 (8)	0.0394 (5)	0.0513 (6)	−0.0082 (5)	0.0287 (5)	−0.0050 (4)
O1	0.130 (3)	0.100 (3)	0.105 (3)	0.063 (3)	0.027 (2)	−0.015 (2)
O2	0.097 (2)	0.099 (3)	0.073 (2)	0.0029 (19)	0.0421 (19)	−0.0249 (19)
O3	0.0549 (16)	0.0571 (17)	0.0818 (19)	−0.0087 (13)	0.0281 (14)	−0.0242 (14)
O4	0.0570 (15)	0.0408 (13)	0.0552 (15)	−0.0032 (12)	0.0236 (12)	−0.0034 (11)
O5	0.0724 (18)	0.0385 (14)	0.0627 (16)	−0.0042 (12)	0.0341 (14)	−0.0075 (11)
N1	0.057 (2)	0.071 (2)	0.078 (3)	0.0045 (18)	0.0303 (19)	−0.016 (2)
N2	0.072 (2)	0.062 (2)	0.0472 (18)	−0.0016 (18)	0.0303 (16)	−0.0028 (16)
C1	0.046 (2)	0.055 (2)	0.059 (2)	0.0014 (18)	0.0188 (18)	−0.0096 (18)
C2	0.052 (2)	0.065 (2)	0.051 (2)	−0.0027 (19)	0.0220 (18)	−0.0049 (19)
C3	0.048 (2)	0.051 (2)	0.062 (2)	0.0034 (18)	0.0134 (18)	0.0034 (19)
C4	0.044 (2)	0.046 (2)	0.066 (2)	−0.0047 (17)	0.0189 (18)	−0.0144 (18)
C5	0.063 (3)	0.069 (3)	0.052 (2)	0.004 (2)	0.0142 (19)	−0.001 (2)
C6	0.059 (2)	0.062 (3)	0.062 (3)	0.016 (2)	0.014 (2)	0.001 (2)
C7	0.064 (2)	0.0289 (18)	0.050 (2)	−0.0006 (17)	0.0199 (17)	−0.0022 (15)
C8	0.075 (3)	0.0382 (19)	0.059 (2)	0.0129 (18)	0.035 (2)	0.0015 (17)
C9	0.061 (2)	0.0342 (18)	0.0402 (18)	0.0061 (15)	0.0211 (16)	0.0001 (14)
C10	0.059 (2)	0.044 (2)	0.048 (2)	−0.0019 (17)	0.0174 (18)	−0.0057 (16)
C11	0.054 (2)	0.052 (2)	0.052 (2)	0.0010 (18)	0.0242 (17)	0.0101 (18)

Geometric parameters (Å, °)

Cl—C11	1.710 (4)	C1—C6	1.375 (5)
S—C9	1.721 (3)	C2—C3	1.380 (6)
S—C11	1.709 (4)	C3—C4	1.370 (5)
O1—N1	1.212 (6)	C4—C5	1.371 (5)
O2—N1	1.219 (5)	C5—C6	1.383 (6)
O3—C4	1.407 (4)	C8—C9	1.489 (5)
O3—C7	1.340 (5)	C9—C10	1.339 (5)
O4—C7	1.189 (4)	C2—H2B	0.9293
O5—C7	1.332 (4)	C3—H3A	0.9306
O5—C8	1.460 (5)	C5—H5A	0.9307
N1—C1	1.459 (6)	C6—H6A	0.9300
N2—C10	1.373 (5)	C8—H8A	0.9700
N2—C11	1.286 (5)	C8—H8B	0.9705
C1—C2	1.377 (6)	C10—H10A	0.9303
C9—S—C11	88.61 (18)	S—C9—C10	108.8 (3)
C4—O3—C7	116.1 (3)	C8—C9—C10	126.1 (3)
C7—O5—C8	115.6 (3)	N2—C10—C9	117.4 (3)
O1—N1—O2	123.4 (4)	Cl—C11—S	120.4 (2)
O1—N1—C1	118.1 (4)	Cl—C11—N2	122.7 (3)
O2—N1—C1	118.5 (4)	S—C11—N2	116.8 (3)
C10—N2—C11	108.4 (3)	C1—C2—H2B	120.54
N1—C1—C2	118.7 (3)	C3—C2—H2B	120.52
N1—C1—C6	119.2 (4)	C2—C3—H3A	120.53
C2—C1—C6	122.1 (4)	C4—C3—H3A	120.49
C1—C2—C3	118.9 (4)	C4—C5—H5A	120.37
C2—C3—C4	119.0 (4)	C6—C5—H5A	120.46
O3—C4—C3	119.4 (3)	C1—C6—H6A	120.59

O3—C4—C5	118.4 (3)	C5—C6—H6A	120.78
C3—C4—C5	122.2 (4)	O5—C8—H8A	109.05
C4—C5—C6	119.2 (3)	O5—C8—H8B	109.10
C1—C6—C5	118.6 (4)	C9—C8—H8A	109.05
O3—C7—O4	126.2 (3)	C9—C8—H8B	109.01
O3—C7—O5	107.1 (3)	H8A—C8—H8B	107.81
O4—C7—O5	126.7 (4)	N2—C10—H10A	121.24
O5—C8—C9	112.7 (3)	C9—C10—H10A	121.35
S—C9—C8	124.9 (3)		
C6—C1—N1—O1	−0.1 (6)	C8—O5—C7—O4	4.4 (5)
C2—C1—N1—O1	179.9 (4)	C8—O5—C7—O3	−174.8 (3)
C6—C1—N1—O2	−178.7 (4)	C4—O3—C7—O4	−0.7 (5)
C2—C1—N1—O2	1.3 (5)	C4—O3—C7—O5	178.6 (3)
C6—C1—C2—C3	0.8 (6)	C7—O5—C8—C9	−82.1 (4)
N1—C1—C2—C3	−179.2 (3)	O5—C8—C9—C10	−99.7 (4)
C1—C2—C3—C4	0.3 (6)	O5—C8—C9—S	84.7 (4)
C2—C3—C4—C5	−0.9 (6)	C11—S—C9—C10	0.0 (3)
C2—C3—C4—O3	−177.8 (3)	C11—S—C9—C8	176.3 (3)
C7—O3—C4—C3	−77.0 (4)	C8—C9—C10—N2	−176.2 (3)
C7—O3—C4—C5	106.1 (4)	S—C9—C10—N2	0.1 (4)
C3—C4—C5—C6	0.5 (6)	C11—N2—C10—C9	−0.2 (5)
O3—C4—C5—C6	177.3 (3)	C10—N2—C11—S	0.2 (4)
C2—C1—C6—C5	−1.3 (6)	C10—N2—C11—Cl	177.6 (3)
N1—C1—C6—C5	178.7 (4)	C9—S—C11—N2	−0.2 (3)
C4—C5—C6—C1	0.6 (6)	C9—S—C11—Cl	−177.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8A···O4^{i}	0.97	2.44	3.392 (4)	166
C8—H8B···N2^{ii}	0.97	2.54	3.325 (5)	138

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2.

Fig. 1

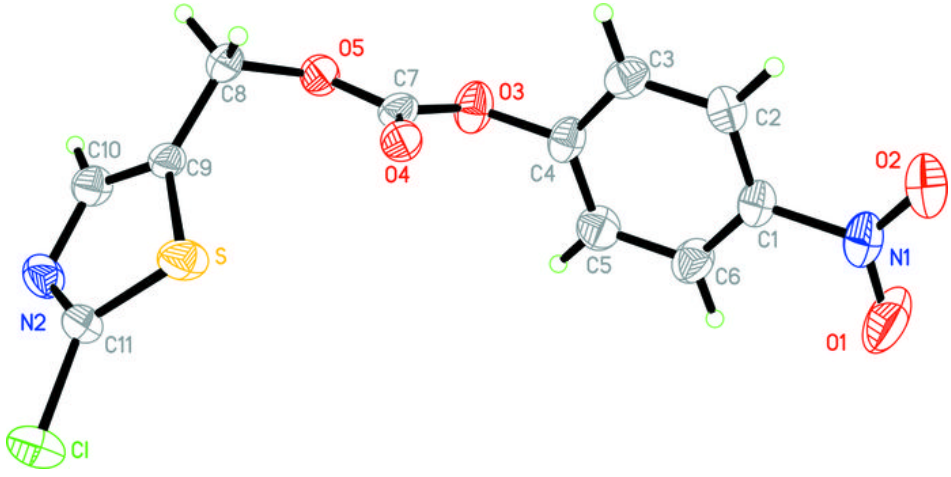

Fig. 2